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ANISOTROPY OF THE OPTICAL ABSORPTION IN $MoSe_2$ SINGLE CRYSTALS

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Abstract

The optical energy gap of $MoSe_2$ single crystal has been measured at room temperature near the fundamental absorption method. The incident light was polarized along c-axis of the crystals. Two and three dimensional models are adopted for generating the results. Direct as well as indirect transitions are involved in the absorption process. The indirect transition was found to be allowed with two phonons involved in the process. The three dimensional model could be used to describe the optical properties of the single crystal of $MoSe_2$.

Keywords : Anisotropy, optical properties; energy band gap; $MoSe_2$ single crystal.

I. INTRODUCTION

During recent years, Transition Metal Dichalcogenides (TMDC) of group IV-b,V-b and VI-b have received considerable attention because of their uses particularly as electrodes in photoelectrochamical (PEC) solar ce1l for conversion of solar energy into electrical energy as well as photonic devices in various electronic applications [1-15]. It is clear from the literature survey that, the work on optical absorption of $MoSe_2$ is almost negligible. Hence, it was decided to work on $MoSe_2$ single crystal. In order to study their photo conversion behavior with their band gaps from an analysis of their absorption spectra. Recently, we have reported the absorption spectra for intercalated and layered single crystals of $MoSe_2$ [1-13]. The present work provides the detailed study of the absorption spectra of $MoSe_2$ single crystal and the results of this investigation is narrated in this paper. Very recently Sumesh *et al.* [14, 15] have been reported specific contact resistance at In-n$MoSe_2$ interfaces and current-voltage-temperature characteristics experimentally.

II.EXPERIMENTAL TECHNIQUES

The single crystal of $MoSe_2$ is grown by direct vapour transport technique. The optical characterization of these crystals for determining the direct and indirect band gap is carried out on UV–VIS-NIR Schimadzu-spectrometer in the range 700 nm to 1450 nm. The measurements were performed at room temperature with the incident beam normal to the basal plane i.e. along the c-axis could not be performed since the specimen were too thin to be mounted along this direction.

III. RESULTS AND DISCUSSION

The absorption spectrum of $MoSe_2$ single crystal was taken the spectral ranges 700 nm to 1450 nm. The results from this spectrum were analyzed on the basis of three as well as two dimensional models. For this purpose, values of absorption coefficient α were determined at every

step of 10 nm from 700 nm to 1450 nm from the spectrum. The interpretation of the results in terms of the direct and indirect transitions can be performed with the help of formulae derived for three dimensional (3D) crystals. We have used here the formulae given by Bardeen *et al.* [16] for three dimensional (3D) crystals.

Figures 1 and 2 show the spectral dependences of the absorptions near the energy gap i.e. $(\alpha h\upsilon)^{1/3}$ and $(\alpha h\upsilon)^{1/2}$ Vs. $E^{'}$, respectively. Since, both the curves indicated discontinuous straight lines it is quite plausible that they represent indirect interband transitions involving the emission or absorption of phonons. However from the Figures 1 and 2 one can see that, it is not possible to fit all the experimental points on this curve. It is therefore conjectured that the indirect transitions represents by the absorption curve is an indirect transition allowed. In order to make an accurate determination of the point of discontinuities in Figures 1 and 2 have followed the method adopted by Elkorashy [17].

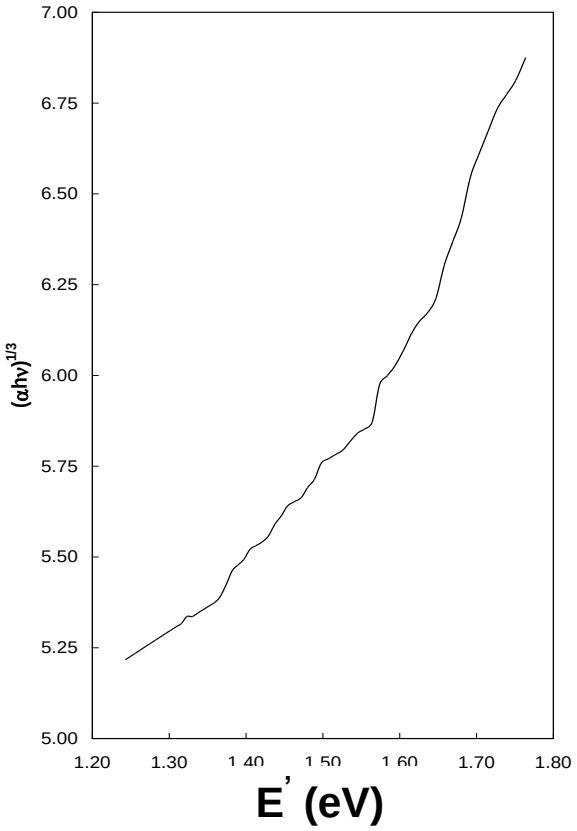

Figure 1: Spectral dependences of the absorption near the energy gap $(\alpha h\nu)^{1/3}$ vs. $E^{'}$ for $MoSe_2$.

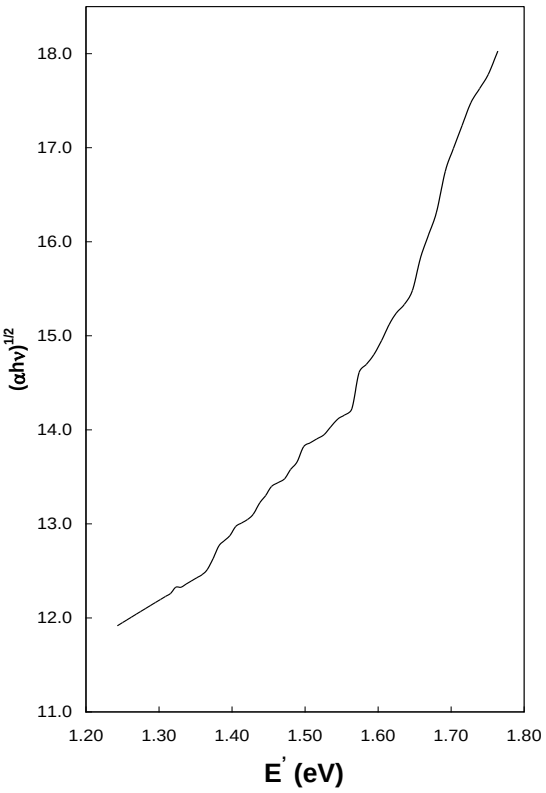

Figure 2 : Spectral dependences of the absorption near the energy gap $(\alpha h\nu)^{1/2}$ vs. E' for $MoSe_2$.

Accordingly from the graphical differentiation of the data presented in Figure 1, we have shown the derivative of the spectral dependences of the absorption near the energy gap i.e. $\delta(\alpha h\upsilon)^{1/2}/\delta E$ on E' in Figure 3. It is clearly seen from this figure that the derivatives are step functions of the energy with four steps well defined in the range i.e. $E_1<E_2<E_3< E_4<E$. The values of E_1, E_2, E_3 and E_4 indicate the points of the discontinuities in the plot of $\delta(\alpha h\upsilon)^{1/2}/\delta E$ vs E' in Figure 3. The indirect energy gap obtained from these values of E_1, E_2, E_3 and E_4 are given by:

$$E' = \frac{E_1 + E_4}{2} = \frac{E_3 + E_2}{2}. \quad (1)$$

and for the phonon energies:

$$E_{pl} = \frac{E_4 - E_1}{2} = \frac{E_3 - E_2}{2}. \quad (2)$$

The value of E' can also be obtained from the intercalation of the linear portion of the graph in Figure 1 with the energy axis. This value is in good agreement with value obtained from equations above.

In order to analyze the data from absorption spectrum on the basis of two dimensional models, we studied the variation of $\alpha^{1/2}$ vs E'. However, it was not possible to fit the experimental results on a straight line. It was therefore conjectured that the two dimensional model does not work in the present case.

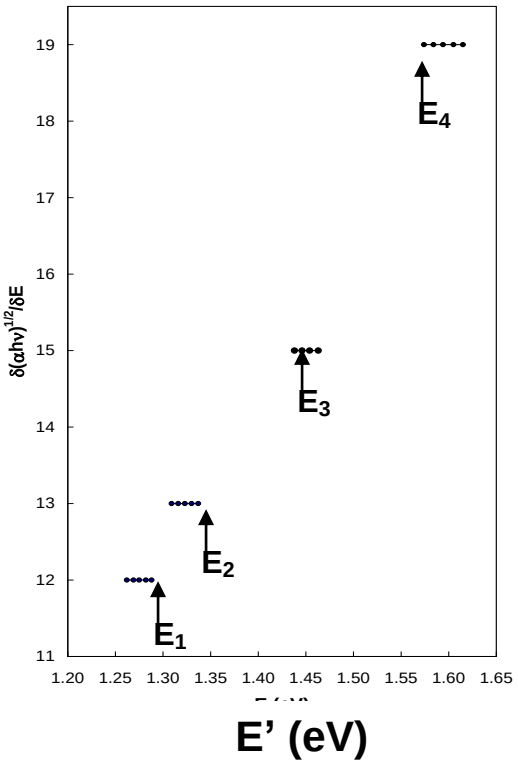

Figure 3: Derivative of the spectral dependences of the absorption near the energy gap $\delta(\alpha h\nu)^{1/2}/\delta E$ vs. $E^{'}$ for $MoSe_2$.

According to theory, for an indirect interband transition, the absorption coefficient can be written as,

$$\alpha = \sum_{l=1}^{2}\left\{ B_{na}\frac{1}{\exp\left(E_{pl}/kT\right)-1}\left(E-E^{'}+E_{pl}\right)^{n} + B_{ne}\frac{1}{1-\exp\left(-E_{pl}/kT\right)}\left(E-E^{'}+E_{pl}\right)^{n}\right\}. \quad (3)$$

where B_{na} and B_{ne} are temperature dependent coefficients representing the processes with phonon absorption and phonon emission, E_{p1} is the energy of the phonon assisting at the transition, n=2 or n=3 for indirect allowed and indirect forbidden transitions. From the expression for E_{p1}, we define a phonon equivalent temperature $\theta_1 = E_{pl}/kT$.

The energy values E_1, E_2, E_3 and E_4 together with indirect energy gap $E^{'}$ as well as two phonon energies Ep_1 and Ep_2 as obtained on the basis of three dimensional indirect (forbidden and allowed) models are shown in Table 1. Knowing the values of hν, $E^{'}$, E_{pl} at room temperature the constants B_{a1}, B_{a2}, B_{e1}, B_{e2}, θ_1, θ_2 have been determined and are also given in Table 1. For the determination of the direct band gap, the best for all the experimental points was observed in the case of $(\alpha h\nu)^2$ vs. $E^{'}$ plot (Figure 4). The values of $E^{'}$ obtained from the intercept of the straight line portion of the hν axis are also shown in Table 1.

The performed experimental measurements of the band energy gap by absorption confirm the three-dimensional features of the layered semiconductors, which were shown by Kolinko *et al.* [18]. Several roles in the specific properties of the absorption may play also

nano-confined effects typical for low-dimensional crystals, which substantially change the band energy dispersions due to flattering of bands [19].

Table 1: Various parameters and constants obtained from the indirect band gap for $MoSe_2$ single crystal.

Parameters	**Indirect (allowed)**	**Direct (allowed)**
E_1 (eV)	1.26	—
E_2 (eV)	1.31	—
E_3 (eV)	1.43	—
E_4 (eV)	1.57	—
$E^{'}$ (eV) C*	1.42 & 1.37	—
E (eV) E*	1.20	—
E (eV)	—	1.47
E_{p1} (meV)	155	—
E_{p2} (meV)	60	—
θ_1 (K)	5.995	—
θ_2 (K)	2.321	—
B_{a1} ($cm^{-1}eV^{-1}$)	68078.85	—
B_{e1} ($cm^{-1}eV^{-1}$)	197.85	—
B_{a2} ($cm^{-1}eV^{-1}$)	2628.00	—
B_{e2} ($cm^{-1}eV^{-1}$)	184.00	—

C* indicates the indirect band gap obtained from calculation and E* indicates the indirect band gap obtained from the extrapolation curve of $(\alpha h\nu)^{1/2}$ vs $E^{'}$.

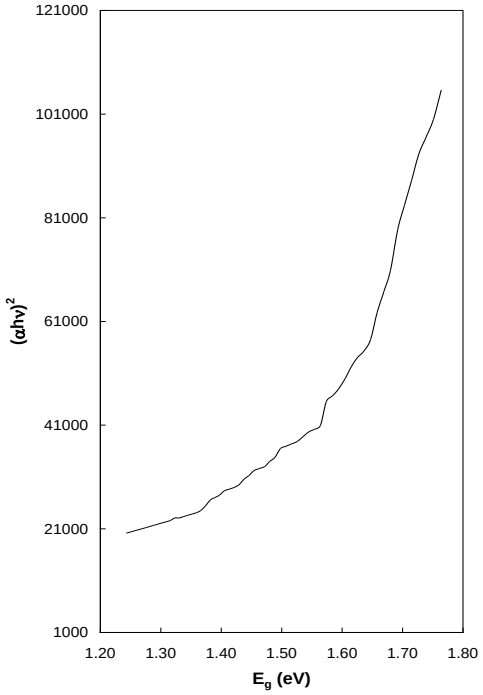

Figure 4: Spectral dependences of the absorption near the energy gap $(\alpha h\nu)^2$ vs. $E^{'}$ for $MoSe_2$.

IV. CONCLUSION

The analysis of accurate measurements of the optical absorption in $MoSe_2$ single crystal has shown that this material possesses both direct as well as indirect band gaps. The phonon assisted indirect transition is indirect allowed. The energies of the phonons have been determined. Further, it is concluded that the two dimensional model cannot be used satisfactorily to describe the main optical properties of this single crystal because it was not possible to fit the experimental results on a straight line. The performed experimental measurements of the band energy gap by absorption confirm the three-dimensional features of the layered semiconductors.

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